WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Oct 21, 2024 – 07:20 AM EDT

PDB ID	:	2B8K
Title	:	12-subunit RNA Polymerase II
Authors	:	Meyer, P.A.; Ye, P.; Zhang, M.; Suh, M.H.; Fu, J.
Deposited on	:	2005-10-07
Resolution	:	4.15 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Clashscore		49
Ramachandran outliers		11.2%
Sidechain outliers		8.6%
RSRZ outliers		13.3%

Worse ← → *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
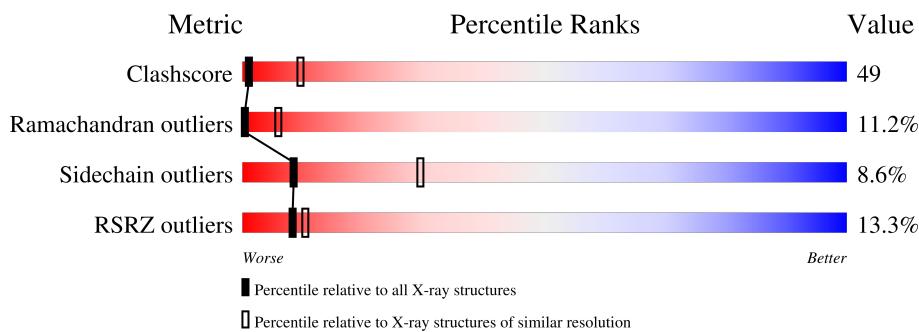
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	180529	1048 (4.50-3.82)
Ramachandran outliers	177936	1231 (4.52-3.80)
Sidechain outliers	177891	1216 (4.52-3.80)
RSRZ outliers	164620	1239 (4.52-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	10% · 27% 43% 10% · 18%
2	B	1224	13% · 29% 48% 12% · 9%
3	C	318	7% · 23% 47% 12% · 16%
4	D	221	14% · 30% 42% 10% 18%
5	E	215	12% · 40% 53% 6%
6	F	155	3% · 17% 31% 6% · 46%
7	G	215	4% · 30% 42% 7% 20%

wwPDB X-ray Structure Validation Summary Report

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Mol	Chain	Length	Quality of chain
8	H	146	23% / 32% / 49% / 10% / 9%
9	I	122	22% / 40% / 43% / 13%
10	J	70	4% / 19% / 51% / 23% / 7%
11	K	120	8% / 41% / 47% / 8%
12	L	70	21% / 13% / 34% / 19% / 34%
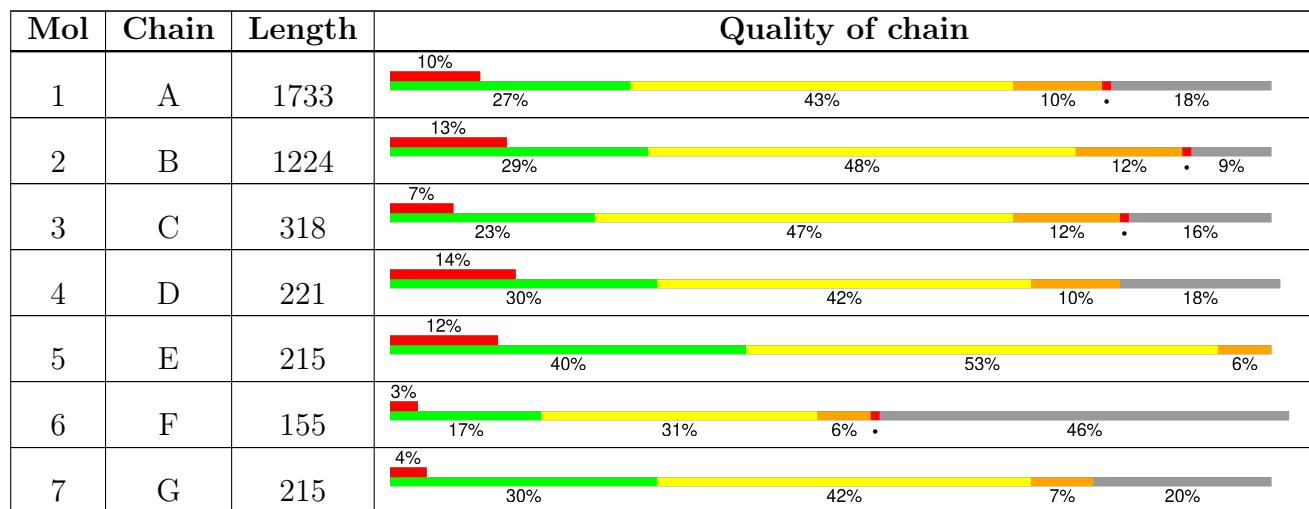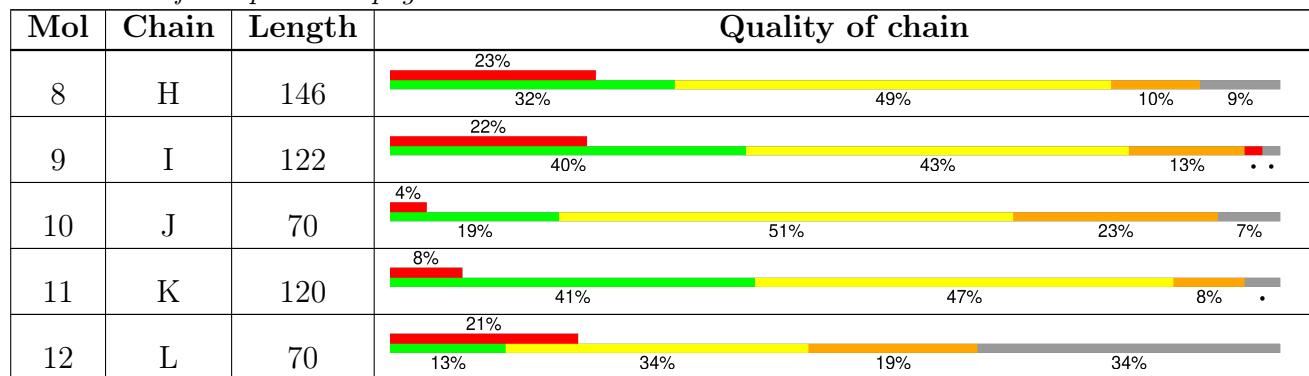
2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 31040 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase II largest subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1416	Total 11140	C 7021	N 1946	O 2111	S 62	0	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1114	Total 8800	C 5573	N 1540	O 1633	S 54	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total 2095	C 1317	N 348	O 417	S 13	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II 32 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	182	Total 1373	C 851	N 243	O 277	S 2	0	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	214	Total 1752	C 1111	N 309	O 321	S 11	0	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	84	Total 679	C 434	N 115	O 127	S 3	0	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II 19 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total 1339	C 861	N 222	O 248	S 8	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	172	SER	-	expression tag	UNP P34087
G	173	HIS	-	expression tag	UNP P34087
G	174	GLU	-	expression tag	UNP P34087
G	175	LYS	-	expression tag	UNP P34087
G	176	ARG	-	expression tag	UNP P34087
G	177	ARG	-	expression tag	UNP P34087
G	178	TRP	-	expression tag	UNP P34087
G	179	LYS	-	expression tag	UNP P34087
G	180	LYS	-	expression tag	UNP P34087
G	181	ASN	-	expression tag	UNP P34087
G	182	PHE	-	expression tag	UNP P34087
G	183	ILE	-	expression tag	UNP P34087
G	184	ALA	-	expression tag	UNP P34087
G	185	VAL	-	expression tag	UNP P34087
G	186	SER	-	expression tag	UNP P34087
G	187	ALA	-	expression tag	UNP P34087
G	188	ALA	-	expression tag	UNP P34087
G	189	ASN	-	expression tag	UNP P34087
G	190	ARG	-	expression tag	UNP P34087
G	191	PHE	-	expression tag	UNP P34087
G	192	LYS	-	expression tag	UNP P34087
G	193	LYS	-	expression tag	UNP P34087
G	194	ILE	-	expression tag	UNP P34087
G	195	SER	-	expression tag	UNP P34087
G	196	SER	-	expression tag	UNP P34087
G	197	SER	-	expression tag	UNP P34087
G	198	GLY	-	expression tag	UNP P34087
G	199	ALA	-	expression tag	UNP P34087
G	200	LEU	-	expression tag	UNP P34087
G	201	ASP	-	expression tag	UNP P34087
G	202	TYR	-	expression tag	UNP P34087

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Chain	Residue	Modelled	Actual	Comment	Reference
G	203	ASP	-	expression tag	UNP P34087
G	204	ILE	-	expression tag	UNP P34087
G	205	PRO	-	expression tag	UNP P34087
G	206	THR	-	expression tag	UNP P34087
G	207	THR	-	expression tag	UNP P34087
G	208	ALA	-	expression tag	UNP P34087
G	209	SER	-	expression tag	UNP P34087
G	210	GLU	-	expression tag	UNP P34087
G	211	ASN	-	expression tag	UNP P34087
G	212	LEU	-	expression tag	UNP P34087
G	213	TYR	-	expression tag	UNP P34087
G	214	PHE	-	expression tag	UNP P34087
G	215	GLN	-	expression tag	UNP P34087

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	133	1068	673	180	211	4	0	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	I	119	971	596	179	186	10	0	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerases I/II/III subunit 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	J	65	532	339	93	94	6	0	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	115	920	590	157	171	2	0	0	1

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	46	363	224	72	63	4	0	0	0

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	2	Total 2	Zn 2	0	0
13	B	1	Total 1	Zn 1	0	0
13	C	1	Total 1	Zn 1	0	0
13	I	2	Total 2	Zn 2	0	0
13	J	1	Total 1	Zn 1	0	0
13	L	1	Total 1	Zn 1	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA-directed RNA polymerase II largest subunit

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THR SER PRO GLY TYR SER GLY SER PRO ALA TYR SER PRO LYS GLN ASP GLU GLN LYS HIS ASN GLU ASN ASN SER ARG

• Molecule 2: DNA-directed RNA polymerase II 140 kDa polypeptide

Chain B:

• Molecule 3: DNA-directed RNA polymerase II 45 kDa polypeptide

• Molecule 4: DNA-directed RNA polymerase II 32 kDa polypeptide

Chain D:
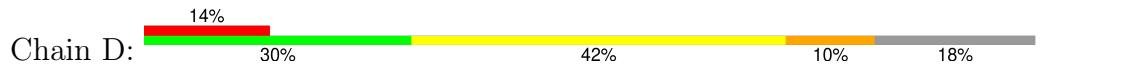
• Molecule 5: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide

Chain E:

• Molecule 6: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

Chain F:
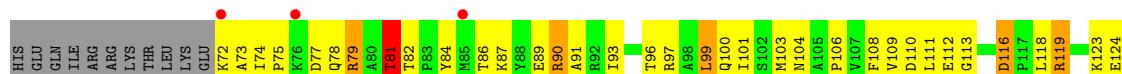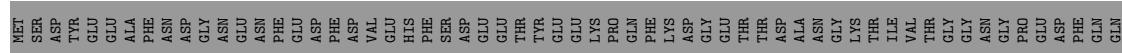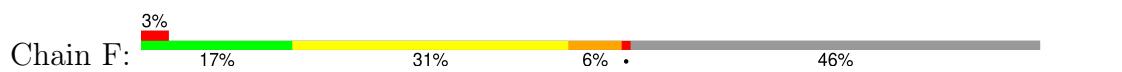
• Molecule 7: DNA-directed RNA polymerase II 19 kDa polypeptide

Chain G:

4%

30%   42%   7%   20%
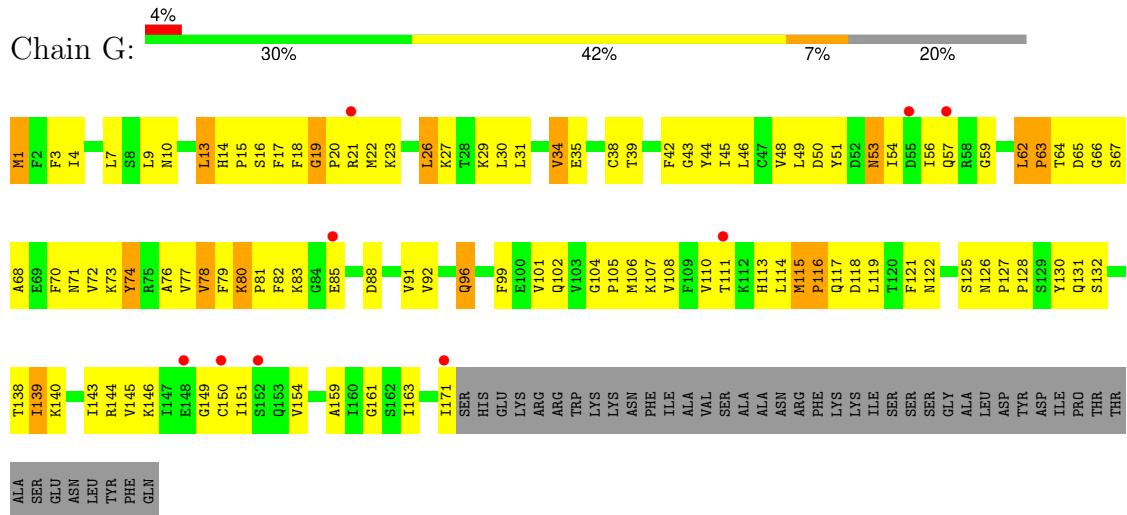
• Molecule 8: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide

Chain H:

23%

32%   49%   10%   9%
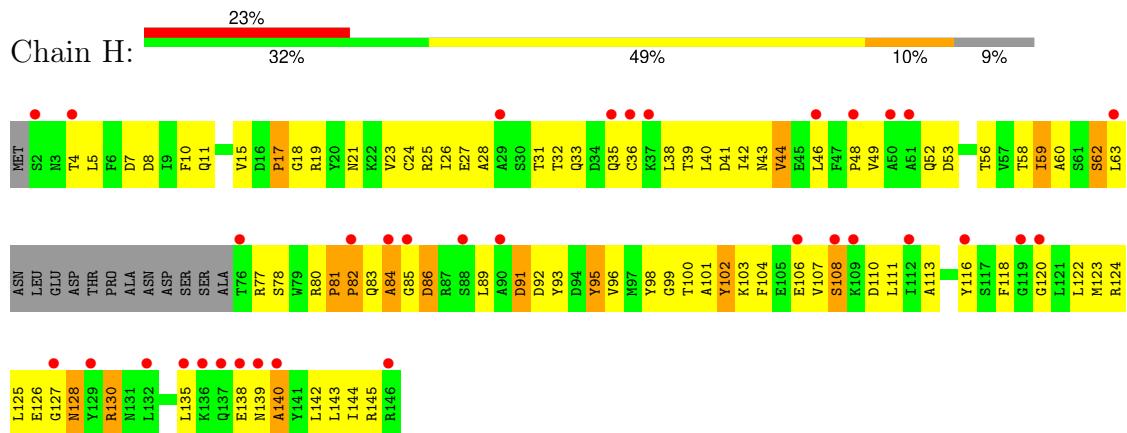
• Molecule 9: DNA-directed RNA polymerase II subunit 9

Chain I:

22%

40%   43%   13%
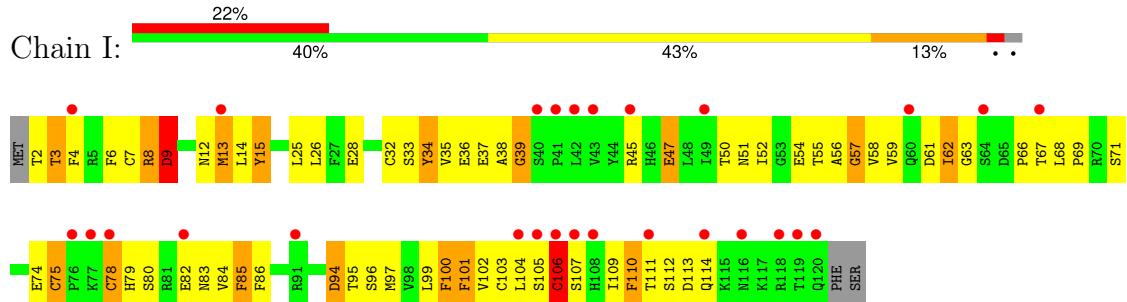
• Molecule 10: DNA-directed RNA polymerases I/II/III subunit 10

Chain J:

4%

19%   51%   23%   7%
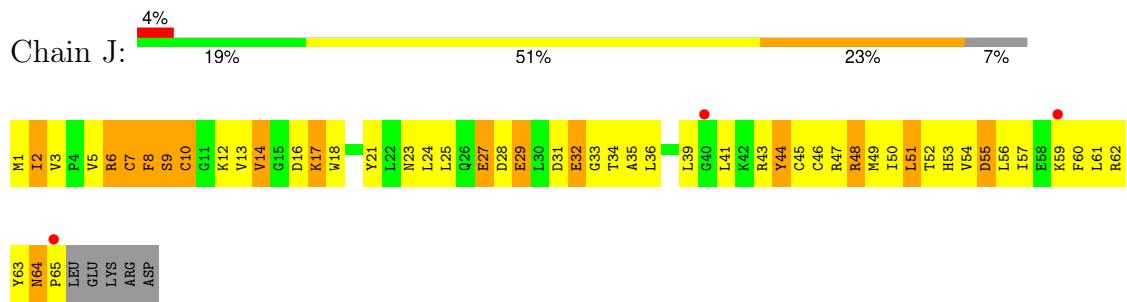
• Molecule 11: DNA-directed RNA polymerase II 13.6 kDa polypeptide

Chain K:
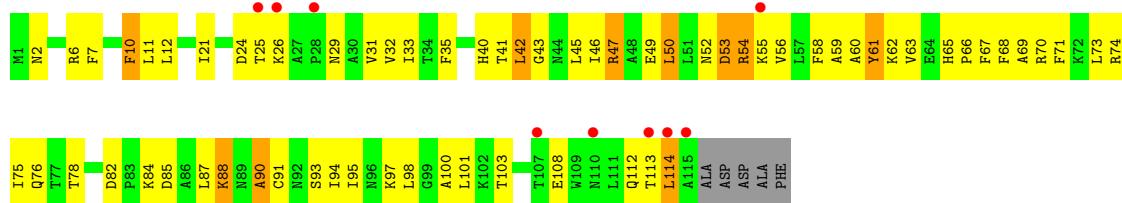
• Molecule 12: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	220.69Å 394.33Å 281.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	158.11 – 4.15 158.11 – 4.15	Depositor EDS
% Data completeness (in resolution range)	(Not available) (158.11-4.15) 83.4 (158.11-4.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 4.15Å)	Xtriage
Refinement program		Depositor
R, R_{free}	0.387 , (Not available) 0.306 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	118.6	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 176.0	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.023 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.023 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	31040	wwPDB-VP
Average B, all atoms (Å^2)	169.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.49	3/11339 (0.0%)	0.75	9/15334 (0.1%)
2	B	0.53	6/8971 (0.1%)	0.97	25/12103 (0.2%)
3	C	0.52	0/2133	0.76	0/2891
4	D	0.49	0/1382	0.81	3/1862 (0.2%)
5	E	0.44	0/1788	0.64	0/2406
6	F	0.53	0/691	0.78	0/933
7	G	0.53	0/1367	0.74	0/1844
8	H	0.40	0/1086	0.66	0/1470
9	I	0.83	1/989 (0.1%)	0.94	3/1331 (0.2%)
10	J	0.54	0/541	0.90	1/727 (0.1%)
11	K	0.50	0/938	0.68	0/1267
12	L	0.55	0/365	0.79	0/485
All	All	0.52	10/31590 (0.0%)	0.82	41/42653 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	1	10
3	C	0	1
9	I	0	1
All	All	1	14

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	39	GLY	C-N	-21.36	0.84	1.34
2	B	442	PHE	C-N	-8.69	1.14	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	446	LEU	N-CA	-8.12	1.30	1.46
2	B	439	ALA	C-N	7.40	1.51	1.34
1	A	1274	ARG	C-N	-6.45	1.21	1.33

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	475	SER	CB-CA-C	-51.20	12.82	110.10
9	I	39	GLY	O-C-N	-18.15	93.66	122.70
2	B	439	ALA	N-CA-CB	-16.49	87.01	110.10
2	B	442	PHE	C-N-CA	15.77	161.13	121.70
2	B	476	ARG	C-N-CA	-15.07	84.02	121.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	475	SER	CA

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	303	TYR	Sidechain
1	A	807	GLY	Mainchain
2	B	217	ARG	Mainchain
2	B	405	ARG	Mainchain
2	B	438	GLU	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11140	0	11218	1169	0
2	B	8800	0	8777	947	0
3	C	2095	0	2053	241	0
4	D	1373	0	1312	144	0
5	E	1752	0	1776	149	0
6	F	679	0	701	94	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1339	0	1357	145	0
8	H	1068	0	1040	107	0
9	I	971	0	929	91	0
10	J	532	0	542	93	0
11	K	920	0	929	83	0
12	L	363	0	387	47	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	0	0
13	J	1	0	0	0	0
13	L	1	0	0	0	0
All	All	31040	0	31021	3039	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 49.

The worst 5 of 3039 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:469:GLN:CA	2:B:474:SER:CB	1.80	1.51
4:D:119:ARG:N	4:D:121:LYS:HB2	1.46	1.30
4:D:113:PHE:CB	4:D:156:ASP:OD1	1.78	1.30
4:D:118:THR:HA	4:D:121:LYS:CB	1.64	1.27
2:B:435:THR:CG2	2:B:439:ALA:HB2	1.63	1.26

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1406/1733 (81%)	949 (68%)	293 (21%)	164 (12%)	0	5
2	B	1096/1224 (90%)	744 (68%)	226 (21%)	126 (12%)	0	5
3	C	264/318 (83%)	159 (60%)	66 (25%)	39 (15%)	0	3
4	D	178/221 (80%)	124 (70%)	35 (20%)	19 (11%)	0	6
5	E	212/215 (99%)	147 (69%)	50 (24%)	15 (7%)	1	13
6	F	82/155 (53%)	64 (78%)	14 (17%)	4 (5%)	2	19
7	G	169/215 (79%)	131 (78%)	26 (15%)	12 (7%)	1	13
8	H	129/146 (88%)	84 (65%)	29 (22%)	16 (12%)	0	4
9	I	117/122 (96%)	79 (68%)	31 (26%)	7 (6%)	1	16
10	J	63/70 (90%)	37 (59%)	10 (16%)	16 (25%)	0	1
11	K	113/120 (94%)	89 (79%)	18 (16%)	6 (5%)	1	18
12	L	44/70 (63%)	19 (43%)	14 (32%)	11 (25%)	0	1
All	All	3873/4609 (84%)	2626 (68%)	812 (21%)	435 (11%)	0	6

5 of 435 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	48	ALA
1	A	54	ASN
1	A	55	ASP
1	A	57	ARG

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1239/1520 (82%)	1135 (92%)	104 (8%)	9	30
2	B	952/1061 (90%)	865 (91%)	87 (9%)	7	26
3	C	234/274 (85%)	212 (91%)	22 (9%)	7	25
4	D	138/200 (69%)	122 (88%)	16 (12%)	4	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	196/197 (100%)	187 (95%)	9 (5%)	23	47
6	F	74/137 (54%)	65 (88%)	9 (12%)	4	18
7	G	152/190 (80%)	142 (93%)	10 (7%)	14	37
8	H	117/128 (91%)	111 (95%)	6 (5%)	20	44
9	I	113/116 (97%)	99 (88%)	14 (12%)	4	18
10	J	60/65 (92%)	54 (90%)	6 (10%)	6	23
11	K	99/102 (97%)	92 (93%)	7 (7%)	12	35
12	L	40/57 (70%)	37 (92%)	3 (8%)	11	33
All	All	3414/4047 (84%)	3121 (91%)	293 (9%)	8	29

5 of 293 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	104	ASN
11	K	47	ARG
6	F	79	ARG
8	H	95	TYR
1	A	1400	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	167	HIS
9	I	12	ASN
3	C	252	GLN
5	E	104	ASN
11	K	65	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
2	B	1
9	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	807:GLY	C	808:LEU	N	1.20
1	B	442:PHE	C	443:ASN	N	1.14
1	I	39:GLY	C	40:SER	N	0.84

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1416/1733 (81%)	1.05	181 (12%)	9	11	96, 165, 229, 265	0
2	B	1114/1224 (91%)	1.03	157 (14%)	7	10	20, 162, 239, 270	0
3	C	266/318 (83%)	0.87	23 (8%)	18	17	114, 157, 215, 237	0
4	D	182/221 (82%)	1.25	32 (17%)	4	7	20, 170, 207, 228	0
5	E	214/215 (99%)	0.96	26 (12%)	10	12	111, 196, 241, 247	0
6	F	84/155 (54%)	0.81	5 (5%)	29	25	109, 143, 189, 209	0
7	G	171/215 (79%)	0.77	9 (5%)	33	28	119, 147, 177, 201	0
8	H	133/146 (91%)	1.38	34 (25%)	2	4	173, 210, 246, 255	0
9	I	119/122 (97%)	1.53	27 (22%)	3	5	104, 200, 236, 277	0
10	J	65/70 (92%)	0.72	3 (4%)	38	31	119, 156, 197, 204	0
11	K	115/120 (95%)	0.85	9 (7%)	20	19	119, 160, 191, 199	0
12	L	46/70 (65%)	1.78	15 (32%)	1	3	153, 214, 245, 253	0
All	All	3925/4609 (85%)	1.04	521 (13%)	8	10	20, 164, 234, 277	0

The worst 5 of 521 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	472	ALA	8.5
1	A	1081	LEU	7.3
4	D	116	SER	6.6
2	B	471	LYS	6.4
2	B	882	THR	6.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	ZN	B	1225	1/1	0.95	0.21	20,20,20,20	0
13	ZN	A	1735	1/1	0.96	0.21	20,20,20,20	0
13	ZN	A	1734	1/1	0.97	0.27	20,20,20,20	0
13	ZN	C	319	1/1	0.98	0.17	20,20,20,20	0
13	ZN	I	124	1/1	0.99	0.25	20,20,20,20	0
13	ZN	L	71	1/1	0.99	0.23	20,20,20,20	0
13	ZN	J	71	1/1	1.00	0.18	20,20,20,20	0
13	ZN	I	123	1/1	1.00	0.20	20,20,20,20	0

6.5 Other polymers ⓘ

There are no such residues in this entry.